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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	OCT 04	Removal of Pre-IPC 8 data fields streamlines displays in USPATFULL, USPAT2, and USPATOLD.
NEWS 3	OCT 04	Precision of EMBASE searching enhanced with new chemical name field
NEWS 4	OCT 06	Increase your retrieval consistency with new formats or for Taiwanese application numbers in CA/CAplus.
NEWS 5	OCT 21	CA/CAplus kind code changes for Chinese patents increase consistency, save time
NEWS 6	OCT 22	New version of STN Viewer preserves custom highlighting of terms when patent documents are saved in .rtf format
NEWS 7	OCT 28	INPADOCDB/INPAFAMDB: Enhancements to the US national patent classification.
NEWS 8	NOV 03	New format for Korean patent application numbers in CA/CAplus increases consistency, saves time.
NEWS 9	NOV 04	Selected STN databases scheduled for removal on December 31, 2010
NEWS 10	NOV 18	PROUSDDR and SYNTHLINE Scheduled for Removal December 31, 2010 by Request of Prous Science
NEWS 11	NOV 22	Higher System Limits Increase the Power of STN Substance-Based Searching
NEWS 12	NOV 22	Enjoy a free month of INPADOCDB/INPAFAMDB SDIs!
NEWS 13	NOV 24	Search an additional 46,850 records with MEDLINE backfile extension to 1946
NEWS 14	DEC 14	New PNK Field Allows More Precise Crossover among STN Patent Databases
NEWS 15	DEC 17	ReaxysFile will replace the Beilstein database
NEWS 16	DEC 21	CAS Learning Solutions -- a new online training experience
NEWS 17	DEC 22	Value-Added Indexing Improves Access to World Traditional Medicine Patents in CAplus

NEWS EXPRESS FEBRUARY 15 10 CURRENT WINDOWS VERSION IS V8.4.2,
AND CURRENT DISCOVER FILE IS DATED 07 JULY 2010.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

products is prohibited and may result in loss of user privileges
and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 17:32:29 ON 27 DEC 2010

=> fil reg

FILE 'REGISTRY' ENTERED AT 17:32:47 ON 27 DEC 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 26 DEC 2010 HIGHEST RN 1257513-11-3
DICTIONARY FILE UPDATES: 26 DEC 2010 HIGHEST RN 1257513-11-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

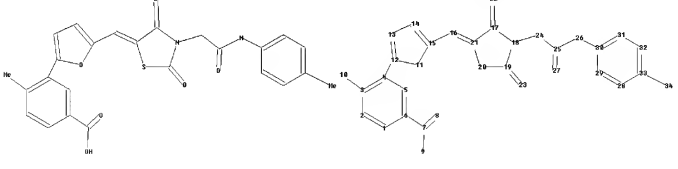
TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10582640 Immunomodulatory Compounds.str



chain nodes :
7 8 9 10 16 22 23 24 25 26 27 34
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 17 18 19 20 21 28 29 30 31 32 33
chain bonds :
3-10 4-12 6-7 7-8 7-9 15-16 16-21 17-22 18-24 19-23 24-25 25-26 25-27
26-30 33-34
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-15 12-13 13-14 14-15 17-18 17-21 18-
19 19-20 20-21 28-29 28-33 29-30 30-31 31-32 32-33
exact/norm bonds :
11-12 11-15 12-13 13-14 14-15 17-18 17-21 17-22 18-19 18-24 19-20 19-23

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20-21  25-26  25-27  26-30
exact bonds :
3-10  4-12  6-7  15-16  16-21  24-25  33-34
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  7-8  7-9  28-29  28-33  29-30  30-31  31-32  32-33


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
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28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  33:Atom  34:CLASS



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 17:33:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       51 TO ITERATE

100.0% PROCESSED       51 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          592 TO     1448
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s sss full l1
FULL SEARCH INITIATED 17:33:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      782 TO ITERATE

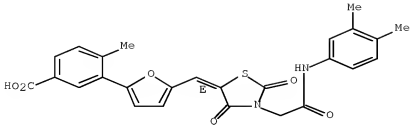
100.0% PROCESSED      782 ITERATIONS                                4 ANSWERS
SEARCH TIME: 00.00.01

L3            4 SEA SSS FUL L1

=> d l3 1-4

L3   ANSWER 1 OF 4  REGISTRY  COPYRIGHT 2010 ACS on STN
RN   1164479-41-7  REGISTRY
ED   Entered STN:  19 Jul 2009
CN   Benzoic acid, 3-[5-[(E)-[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-
     dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl-  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C26 H22 N2 O6 S
SR   CA
LC   STN Files:   CA, CAPLUS, CHEMCATS
```

Double bond geometry as shown.

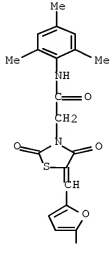


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

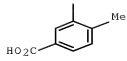
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 2 OF 4 REGISTRY COPYRIGHT 2010 ACS on STN
RN 866243-78-9 REGISTRY
ED Entered STN: 27 Oct 2005
CN Benzoic acid, 3-[5-[[2,4-dioxo-3-[2-oxo-2-[(2,4,6-trimethylphenyl)amino]ethyl]-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)
MF C27 H24 N2 O6 S
SR Chemical Library
Supplier: TimTec, Inc.

PAGE 1-A



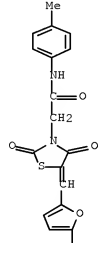
PAGE 2-A



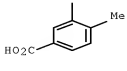
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 ANSWER 3 OF 4 REGISTRY COPYRIGHT 2010 ACS on STN
RN 496767-24-9 REGISTRY
ED Entered STN: 03 Mar 2003
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)
MF C25 H20 N2 O6 S
SR Chemical Library
Supplier: Interchim
LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER, USPATFULL

PAGE 1-A



PAGE 2-A



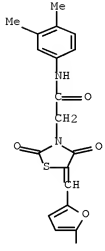
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)

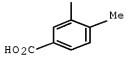
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 4 OF 4 REGISTRY COPYRIGHT 2010 ACS on STN
RN 431986-92-4 REGISTRY
ED Entered STN: 19 Jun 2002
CN Benzoic acid, 3-[5-[[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)
MF C26 H22 N2 O6 S
SR Chemical Library
Supplier: ChemBridge Corporation
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus uspatfull toxcenter

FILE 'CAPLUS' ENTERED AT 17:34:47 ON 27 DEC 2010
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```
FILE 'USPATFULL' ENTERED AT 17:34:47 ON 27 DEC 2010
CA INDEXING COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'TOXCENTER' ENTERED AT 17:34:47 ON 27 DEC 2010
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

=> d hist

     (FILE 'HOME' ENTERED AT 17:32:29 ON 27 DEC 2010)

     FILE 'REGISTRY' ENTERED AT 17:32:47 ON 27 DEC 2010
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           4 S SSS FULL L1

     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 17:34:47 ON 27 DEC 2010

=> s l3
L4           9 L3

=> dup remove l4
PROCESSING COMPLETED FOR L4
L5           7 DUP REMOVE L4 (2 DUPLICATES REMOVED)

=> d ibib abs hitstr 1-7

L5   ANSWER 1 OF 7  CAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2009:875997  CAPLUS Full-text
DOCUMENT NUMBER:          151:115085
TITLE:                    Method using lifespan-altering compounds for altering
                          the lifespan of eukaryotic organisms, and screening
                          for such compounds
INVENTOR(S):              Goldfarb, David Scott
PATENT ASSIGNEE(S):       University of Rochester, USA
SOURCE:                   U.S. Pat. Appl. Publ., 57pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   20
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ----------------    ----   --------    --------------------   --------
     US 20090163545       A1    20090625    US 2008-341615         20081222
     US 20090163545       A1    20090625    US 2008-341615         20081222
     AU 2008345225        A1    20090709    AU 2008-345225         20081222
     CA 2709784           A1    20090709    CA 2008-2709784        20081222
     EP 2219646           A2    20100825    EP 2008-867410         20081222
         R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU,
             IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI,
             SK, TR, AL, BA, MK, RS
PRIORITY APPLN. INFO.:                          US 2008-23801P      P  20080125
                                                US 2007-16362P      P  20071221
                                                US 2008-341615         20081222
                                                WO 2008-US88016     W  20081222
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
AB   The invention discloses a method for altering the lifespan of a eukaryotic
     organism.  The method comprises the steps of providing a lifespan-altering
     compound, and administering an effective amount of the compound to a
     eukaryotic organism, such that the lifespan of the organism is altered.  In
```

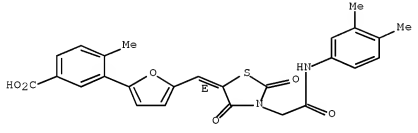
one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 1164479-41-7
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 1164479-41-7 CAPLUS

CN Benzoic acid, 3-[5-[(E)-[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 2 OF 7 USPATFULL on STN

ACCESSION NUMBER:	2007:224298 USPATFULL Full-text		
TITLE:	Immunomodulatory compounds that target and inhibit the py'binding site of tyrosene kinase p56 lck sh2 domain		
INVENTOR(S):	Mackerell, Alexander, Baltimore, MD, UNITED STATES Hayashi, Jun, Ellicott City, MD, UNITED STATES Nagarsekar, Ashish, Gaithersburg, MD, UNITED STATES Huang, Niu, San Francisco, CA, UNITED STATES Macias, Alba, Cambridge, UNITED KINGDOM		
	NUMBER	KIND	DATE
PATENT INFORMATION:	US 20070196395	A1	20070823
APPLICATION INFO.:	US 2003-582640	A1	20031212 (10)
	WO 2003-US39501		20031212
			20070420 PCT 371 date
DOCUMENT TYPE:	Utility		
FILE SEGMENT:	APPLICATION		
LEGAL REPRESENTATIVE:	MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON BLVD., SUITE 1400, ARLINGTON, VA, 22201, US		
NUMBER OF CLAIMS:	23		
EXEMPLARY CLAIM:	1		
NUMBER OF DRAWINGS:	2 Drawing Page(s)		
LINE COUNT:	2189		

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

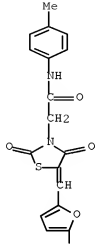
AB Small molecular-weight non-peptidic compounds block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

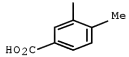
IT 496767-24-9
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)

RN 496767-24-9 USPATFULL
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:1291759 CAPLUS Full-text
DOCUMENT NUMBER: 146:180013
TITLE: Multiplexed Detection of Protein-Peptide Interaction and Inhibition Using Capillary Electrophoresis
AUTHOR(S): Yang, Peilin; Whelan, Rebecca J.; Mao, Yingwei; Lee, Angel W.-M.; Carter-Su, Christin; Kennedy, Robert T.
CORPORATE SOURCE: Department of Chemistry and Department of Pharmacology, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Analytical Chemistry (2007), 79(4), 1690-1695
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-speed capillary electrophoresis (CE) was employed to detect binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes. Single SH2 protein-phosphopeptide complexes were detected and confirmed by competition and fluorescence anisotropy. The assay was then extended to a multiplexed system involving separation of three SH2 domain proteins: Src, SH2-Bβ, and Fyn. The selectivity of the separation was

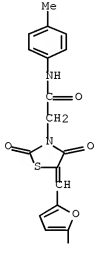
improved by altering the charge of the peptide binding partners used, thus demonstrating a convenient way to control resolution for the multiplexed assay. The separation was completed within 6 s, allowing rapidly dissociating complexes to be detected. Two low mol. weight inhibitors were tested for inhibition selectivity and efficacy. One inhibitor interrupted binding interaction of all three proteins, while the other selectively inhibited Src only leaving SH2-Bβ and Fyn complex barely affected. IC50 of both selective and nonselective inhibitors were determined and compared for different proteins. The IC50 of the nonselective inhibitor was 49±9, 323±42, and 228±19 μM (n = 3) for Src, SH2-Bβ, and Fyn, resp., indicating different efficacy of the nonselective inhibitor for different SH2 domain protein. It is concluded that high-speed CE has the potential for multiplexed screening of drugs that disrupt protein-protein interactions.

IT 496767-24-9
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(high-speed capillary electrophoresis for multiplexed detection of binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes)

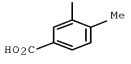
RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2006:1342378 CAPLUS Full-text
DOCUMENT NUMBER: 146:68774
TITLE: Anti-viral compositions comprising heterocyclic substituted phenyl furans and related compounds
INVENTOR(S): Jiang, Shibo; Debnath, Asim Kumar; Lu, Hong
PATENT ASSIGNEE(S): New York Blood Center, USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287319	A1	20061221	US 2006-448439	20060606
CA 2608821	A1	20061228	CA 2006-2608821	20060606
WO 2006138118	A2	20061228	WO 2006-US21993	20060606
WO 2006138118	A3	20070726		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1896033	A2	20080312	EP 2006-772346	20060606
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
JP 2008543836	T	20081204	JP 2008-516935	20060606
PRIORITY APPLN. INFO.:			US 2005-691120P P	20050615
			WO 2006-US21993 W	20060606

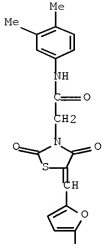
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:68774
AB A group of compds. that inhibit HIV replication by blocking HIV entry was identified. One representative compound, designated NB-206, and its analogs inhibited HIV replication (p24 production) with IC50 values at nanomolar levels. It was proved that NB-206 and its analogs are HIV entry inhibitors by targeting the HIV gp41 since: (1) they inhibited HIV-mediated cell fusion; (2) they inhibited HIV replication only when they were added to the cells less than one hour after virus addition; (3) they blocked the formation of the gp41 core that is detected by sandwich enzyme linked immunosorbent assay (ELISA) using a conformation-specific MAb NC-1; and (4) they inhibited the formation of the gp41 six-helix bundle revealed by fluorescence native-PAGE (FN-PAGE). These results suggested that NB-206 and its analogs may interact with the hydrophobic cavity and block the formation of the fusion-active gp41 coiled coil domain, resulting in inhibition of HIV-1 mediated membrane fusion and virus entry.
IT 431986-92-4
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(anti-viral compns. comprising heterocyclic substituted Ph furans and related compds.)

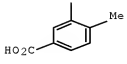
RN 431986-92-4 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2005:588651 CAPLUS Full-text

DOCUMENT NUMBER: 143:109784

TITLE: Immunomodulatory compounds that target and inhibit the py+3 binding site of tyrosine kinase p56lck SH2 domain

INVENTOR(S): Mackerell, Alexander D., Jr.; Hayashi, Jun; Nagarsekar, Ashish; Huang, Niu; Macias, Alba

PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA

SOURCE: PCT Int. Appl., 213 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2005060956 A1 20050707 WO 2003-US39501 20031212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2003297904 A1 20050714 AU 2003-297904 20031212
US 20070196395 A1 20070823 US 2007-582640 20070420
PRIORITY APPLN. INFO.: WO 2003-US39501 A 20031212
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:109784

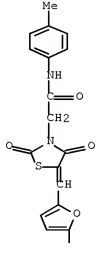
AB Small mol.-wt. non-peptidic compds. block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

IT 496767-24-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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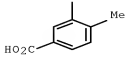

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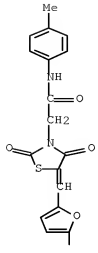
L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1046388 CAPLUS Full-text
DOCUMENT NUMBER: 143:398889
TITLE: Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p56lck
AUTHOR(S): Macias, Alba T.; Mia, Md. Younus; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Chemical Information and Modeling (2005), 45(6), 1759-1766
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Compd. selection based on chem. similarity has been used to validate active "parent" compds. identified via database searching as viable lead compds. and to obtain initial structure-activity relationships for those leads. Twelve parent compds. that have inhibitory activity against the SH2 domain of the p56 T-cell tyrosine kinase (Lck) are the focus of this study. Lck is involved in the T-cell mediated immune response, and inhibitors of Lck protein-protein interactions could potentially be used to develop novel immunosuppressants. Similarity searches for each parent compound were performed using 2D structural fingerprints on a database containing 1 300 000 com. available compds. The inhibitory activity of the selected compds. was assessed using enzyme immunoassay (EIA). In general, the most active parent compds. yield the most high activity similar compds.; however, in two cases low activity parent compds. (i.e.inhibitory activity < 25% at 100 μM) yielded multiple similar compds. with activities > 60%. Such compds. may, therefore, be considered as viable lead compds. for optimization. Structure-activity relationships were explored by examining both ligand structures and their computed bound conformations to the protein. Functional groups common to the active compds. as well as key amino acid residues that form hydrogen bonds with the active compds. were identified. This information will act as the basis for the rational optimization of the lead compds.

IT 496767-24-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lead validation and SAR development via chemical similarity searching; application to compds. targeting pY+3 site of p56lck SH2 domain)
RN 496767-24-9 CAPLUS
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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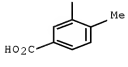

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REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:453664 CAPLUS Full-text
DOCUMENT NUMBER: 141:98930
TITLE: Identification of non-phosphate-containing small molecular weight inhibitors of the tyrosine kinase p56 Lck SH2 domain via in silico screening against the pY + 3 binding site
AUTHOR(S): Huang, Niu; Nagarsekar, Ashish; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(14), 3502-3511
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The protein p56 lymphoid T cell tyrosine kinase (Lck) is predominantly expressed in T lymphocytes where it plays a critical role in T-cell-mediated immune response. Lck participates in phosphotyrosine-dependent protein-protein interactions through its modular binding unit, the Src homol.-2 (SH2)

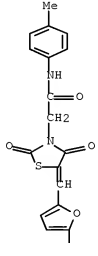
domain. Accordingly, virtual screening methods combined with exptl. assays were used to identify small mol. weight nonpeptidic compds. that block Lck SH2 domain-dependent interactions. Virtual screening included scoring normalization procedures and postdocking structural clustering that is shown to facilitate the selection of active compds. By targeting the well-defined hydrophobic binding pocket known to impart specificity on Lck-protein interactions (i.e., pY + 3 site), inhibitors of the Lck SH2 domain were discovered that omit the phosphotyrosine (pY) or related moieties. The 34 out of 196 computationally selected compds. were shown to inhibit Lck SH2 domain association with phosphorylated immunoreceptor tyrosine based activation motifs peptide. Twenty-four of the active compds. were further tested for their ability to modulate biol. function. Thirteen of these compds. showed inhibitory activity in mixed lymphocyte culture assay. Fluorescence titration expts. on four of these active compds. further verified their binding to the SH2 domain. Because of their simple chemical structures, these small organic compds. have the potential to act as lead compds. for the development of novel immunosuppressant drugs.

IT 496767-24-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of non-phosphate-containing small mol. weight inhibitors of tyrosine kinase p56 Lck SH2 domain via in silico screening against pY + 3 binding site)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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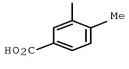

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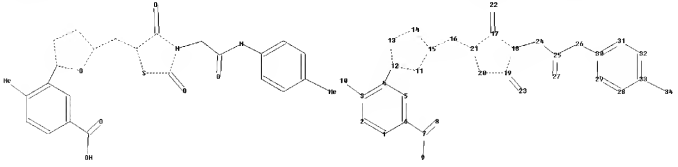

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ring nodes :
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ring bonds :
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exact/norm bonds :
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exact bonds :
3-10 4-12 6-7 24-25 33-34
normalized bonds :
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L6 STRUCTURE UPLOADED

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L6 HAS NO ANSWERS
L6 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> fil reg

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FILE 'REGISTRY' ENTERED AT 17:42:18 ON 27 DEC 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 DEC 2010  HIGHEST RN 1257513-11-3
DICTIONARY FILE UPDATES:  26 DEC 2010  HIGHEST RN 1257513-11-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2010.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l6
SAMPLE SEARCH INITIATED 17:42:22 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       51 TO ITERATE

100.0% PROCESSED       51 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          592 TO     1448
PROJECTED ANSWERS:               0 TO        0

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FULL SCREEN SEARCH COMPLETED -      782 TO ITERATE

100.0% PROCESSED      782 ITERATIONS                               4 ANSWERS
SEARCH TIME: 00.00.01

L8            4 SEA SSS FUL L6

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L3            4 S SSS FULL L1

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L6                STRUCTURE UPLOADED

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L7              0 S L6
L8              4 S L6 SSS FULL

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L10             4 L8 OR L3

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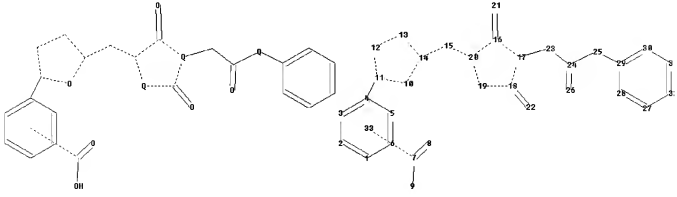

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exact bonds :
4-11  23-24
normalized bonds :
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Match level :
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L11     STRUCTURE UPLOADED

=> s l11
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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 6 TO 266

L12 6 SEA SSS SAM L11

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SEARCH TIME: 00.00.01

L13 91 SEA SSS FUL L11

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L12 ANSWER 1 OF 6 REGISTRY COPYRIGHT 2010 ACS on STN
RN 1025122-48-8 REGISTRY
ED Entered STN: 03 Jun 2008
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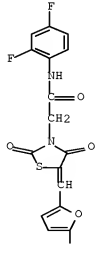
SR Other Sources
Database: ChemDB (University of California Irvine)



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ED Entered STN: 10 Jan 2005
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LC STN Files: CHEMCATS

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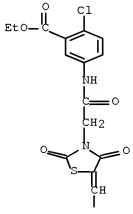

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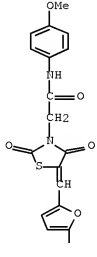
Supplier: Vitas-M
LC STN Files: CHEMCATS

PAGE 1-A



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ED Entered STN: 18 Jun 2002
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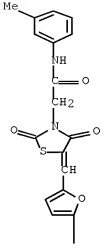
SR Chemical Library
Supplier: ChemBridge Corporation
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL

PAGE 1-A



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RN 431883-68-0 REGISTRY
ED Entered STN: 18 Jun 2002
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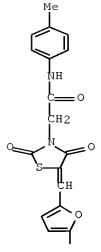
PAGE 1-A



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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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RN 430470-21-6 REGISTRY
ED Entered STN: 14 Jun 2002
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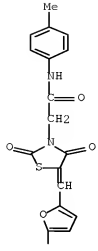
LC STN Files: CA, CAPLUS, CHEMCATS, USPATFULL

PAGE 1-A



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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> fil caplus uspatfull

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FILE 'USPATFULL' ENTERED AT 17:51:20 ON 27 DEC 2010
CA INDEXING COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)

=> d hist

(FILE 'HOME' ENTERED AT 17:32:29 ON 27 DEC 2010)

FILE 'REGISTRY' ENTERED AT 17:32:47 ON 27 DEC 2010
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L2 0 S L1
L3 4 S SSS FULL L1

FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 17:34:47 ON 27 DEC 2010

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L4             9 S L3
L5             7 DUP REMOVE L4 (2 DUPLICATES REMOVED)
L6               STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 17:42:18 ON 27 DEC 2010
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L8             4 S L6 SSS FULL
L9             0 S L8 NOT L3
L10            4 S L8 OR L3
L11              STRUCTURE UPLOADED
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     FILE 'CAPLUS, USPATFULL' ENTERED AT 17:51:20 ON 27 DEC 2010

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=> d hist

     (FILE 'HOME' ENTERED AT 17:32:29 ON 27 DEC 2010)

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L1               STRUCTURE UPLOADED
L2             0 S L1
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L4             9 S L3
L5             7 DUP REMOVE L4 (2 DUPLICATES REMOVED)
L6               STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 17:42:18 ON 27 DEC 2010
L7             0 S L6
L8             4 S L6 SSS FULL
L9             0 S L8 NOT L3
L10            4 S L8 OR L3
L11              STRUCTURE UPLOADED
L12            6 S L11
L13           91 S L11 SSS FULL

     FILE 'CAPLUS, USPATFULL' ENTERED AT 17:51:20 ON 27 DEC 2010
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=> s l15 not l8
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=> s l15 not l3
L17           2 L15 NOT L3

=> d ibib abs hitstr 1-2

L17  ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2008:581012  CAPLUS Full-text
DOCUMENT NUMBER:          149:69549
```

TITLE: Discovery of a novel submicromolar inhibitor of the lymphoid specific tyrosine phosphatase

AUTHOR(S): Xie, Yuli; Liu, Yidong; Gong, Gangli; Rinderspacher, Alison; Deng, Shi-Xian; Smith, Deborah H.; Toebben, Udo; Tzilianos, Effie; Branden, Lars; Vidovic, Dusica; Chung, Caty; Schurer, Stephan; Tautz, Lutz; Landry, Donald W.

CORPORATE SOURCE: Department of Medicine, Columbia University, New York, NY, 10032, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2840-2844
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:69549

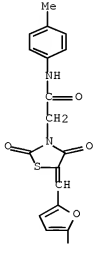
AB We report here a class of thiazolidine-2,4-diones and 2-thioxothiazolidin-4-ones as potent inhibitors of the lymphoid specific tyrosine phosphatase (Lyp) identified from high throughput screens. Chemical modification by incorporating the known phosphotyrosine (pTyr) mimics led to the discovery of a salicylate-based inhibitor with submicromolar potency.

IT 431883-68-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thiazolidinediones and thioxothiazolidinones as inhibitors of lymphoid specific tyrosine phosphatase)

RN 431883-68-0 CAPLUS

CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
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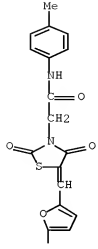
L17 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2007:484949 CAPLUS Full-text
DOCUMENT NUMBER: 146:475681
TITLE: Immunomodulatory heterocyclic compounds that target and inhibit the pY binding site of tyrosine kinase p56lck SH2 domain
INVENTOR(S): Mackerell, Alexander; Hayashi, Jun
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA
SOURCE: U.S. Pat. Appl. Publ., 90 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070099970	A1	20070503	US 2006-507038	20060821
WO 2008024759	A2	20080228	WO 2007-US76402	20070821
WO 2008024759	A3	20081030		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-709972P P 20050819
US 2006-507038 A 20060821
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:475681
AB Small mol.-wt. non-peptidic compds. block lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.
IT 430470-21-6 431883-68-0 431938-97-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory heterocyclic compound inhibitors of pY binding site of tyrosine kinase p56lck SH2 domain)
RN 430470-21-6 CAPLUS
CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

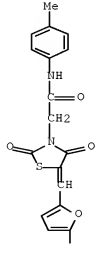
PAGE 1-A



PAGE 2-A

RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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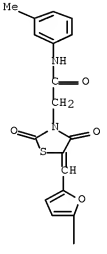
RN 431938-97-5 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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(FILE 'HOME' ENTERED AT 17:32:29 ON 27 DEC 2010)

FILE 'REGISTRY' ENTERED AT 17:32:47 ON 27 DEC 2010
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 4 S SSS FULL L1

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     FILE 'CAPLUS, USPATFULL, TOXCENTER' ENTERED AT 17:34:47 ON 27 DEC 2010
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L5             7 DUP REMOVE L4 (2 DUPLICATES REMOVED)
L6               STRUCTURE UPLOADED

     FILE 'REGISTRY' ENTERED AT 17:42:18 ON 27 DEC 2010
L7             0 S L6
L8             4 S L6 SSS FULL
L9             0 S L8 NOT L3
L10            4 S L8 OR L3
L11              STRUCTURE UPLOADED
L12            6 S L11
L13           91 S L11 SSS FULL

     FILE 'CAPLUS, USPATFULL' ENTERED AT 17:51:20 ON 27 DEC 2010
L14            6 S L12
L15            4 DUP REMOVE L14 (2 DUPLICATES REMOVED)
L16            2 S L15 NOT L8
L17            2 S L15 NOT L3

=> s l13
L18         13 L13

=> dup remove l18
PROCESSING COMPLETED FOR L18
L19           10 DUP REMOVE L18 (3 DUPLICATES REMOVED)

=> d ibib abs hitstr 1-10

L19  ANSWER 1 OF 10  CAPLUS  COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2009:875997  CAPLUS Full-text
DOCUMENT NUMBER:          151:115085
TITLE:                    Method using lifespan-altering compounds for altering
                          the lifespan of eukaryotic organisms, and screening
                          for such compounds
INVENTOR(S):              Goldfarb, David Scott
PATENT ASSIGNEE(S):       University of Rochester, USA
SOURCE:                   U.S. Pat. Appl. Publ., 57pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   20
PATENT INFORMATION:

     PATENT NO.            KIND   DATE        APPLICATION NO.          DATE
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     US 20090163545         A1    20090625    US 2008-341615           20081222
     US 20090163545         A1    20090625    US 2008-341615           20081222
     AU 2008345225          A1    20090709    AU 2008-345225           20081222
     CA 2709784             A1    20090709    CA 2008-2709784          20081222
     EP 2219646             A2    20100825    EP 2008-867410           20081222
          R:  AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU,
              IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI,
              SK, TR, AL, BA, MK, RS
PRIORITY APPLN. INFO.:                        US 2008-23801P      P  20080125
                                              US 2007-16362P      P  20071221
                                              US 2008-341615         20081222
                                              WO 2008-US88016     W  20081222
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
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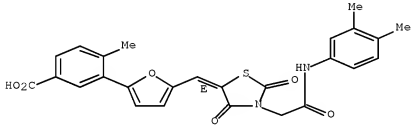
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]

IT 1164479-41-7
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)

RN 1164479-41-7 CAPLUS

CN Benzoic acid, 3-[5-[(E)-[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)

Double bond geometry as shown.



L19 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:825465 CAPLUS Full-text

DOCUMENT NUMBER: 151:235704

TITLE: Identification of Novel Falcipain-2 Inhibitors as Potential Antimalarial Agents through Structure-Based Virtual Screening

AUTHOR(S): Li, Honglin; Huang, Jin; Chen, Lili; Liu, Xiaofeng; Chen, Tong; Zhu, Jin; Lu, Weiqiang; Shen, Xu; Li, Jian; Hilgenfeld, Rolf; Jiang, Hualiang

CORPORATE SOURCE: School of Pharmacy, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China

SOURCE: Journal of Medicinal Chemistry (2009), 52(15), 4936-4940
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

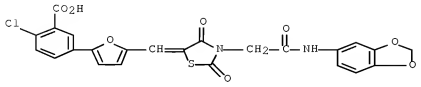
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The SPECS database was screened against falcipain-2 with two different docking methods to identify structurally diverse nonpeptidic inhibitors. Twenty-eight nonpeptidic mols. among 81 compds. tested were identified as potential inhibitors of falcipain-2. One of the inhibitors exhibited in vitro activity with an IC50 value of 2.4 μM. Furthermore, the similarity anal. has demonstrated that it is feasible to find novel diverse falcipain-2 inhibitors with similar steric shape through virtual screening of large-scale chemical libraries.

IT 592540-03-9
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of novel falcipain-2 inhibitors as potential

antimalarial agents through virtual screening)
RN 592540-03-9 CAPLUS
CN Benzoic acid, 5-[5-[[3-[2-(1,3-benzodioxol-5-ylamino)-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)



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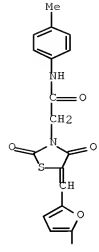
L19 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:581012 CAPLUS Full-text
DOCUMENT NUMBER: 149:69549
TITLE: Discovery of a novel submicromolar inhibitor of the lymphoid specific tyrosine phosphatase
AUTHOR(S): Xie, Yuli; Liu, Yidong; Gong, Gangli; Rinderspacher, Alison; Deng, Shi-Xian; Smith, Deborah H.; Toebben, Udo; Tzilianos, Effie; Branden, Lars; Vidovic, Dusica; Chung, Caty; Schurer, Stephan; Tautz, Lutz; Landry, Donald W.
CORPORATE SOURCE: Department of Medicine, Columbia University, New York, NY, 10032, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2840-2844
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:69549
AB We report here a class of thiazolidine-2,4-diones and 2-thioxothiazolidin-4-ones as potent inhibitors of the lymphoid specific tyrosine phosphatase (Lyp) identified from high throughput screens. Chemical modification by incorporating the known phosphotyrosine (pTyr) mimics led to the discovery of a salicylate-based inhibitor with submicromolar potency.
IT 431883-68-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thiazolidinediones and thioxothiazolidinones as inhibitors of lymphoid specific tyrosine phosphatase)
RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2007:484949 CAPLUS Full-text
DOCUMENT NUMBER: 146:475681
TITLE: Immunomodulatory heterocyclic compounds that target and inhibit the pY binding site of tyrosine kinase p56lck SH2 domain
INVENTOR(S): Mackerell, Alexander; Hayashi, Jun
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA
SOURCE: U.S. Pat. Appl. Publ., 90 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070099970	A1	20070503	US 2006-507038	20060821
WO 2008024759	A2	20080228	WO 2007-US76402	20070821
WO 2008024759	A3	20081030		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI,

GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG,
KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME,
MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL,
PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
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BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-709972P P 20050819
US 2006-507038 A 20060821

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 146:475681

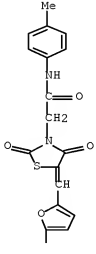
AB Small mol.-wt. non-peptidic compds. block lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

IT 430470-21-6 430471-43-5 431075-18-2
431883-68-0 431883-95-3 431885-49-3
431914-42-0 431938-97-5 432017-78-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory heterocyclic compound inhibitors of pY binding site of tyrosine kinase p56lck SH2 domain)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

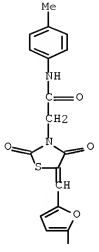
PAGE 1-A



PAGE 2-A

RN 430471-43-5 CAPLUS
CN Benzoic acid, 2-chloro-4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 431075-18-2 CAPLUS
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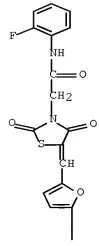
PAGE 1-A



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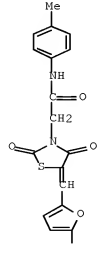
RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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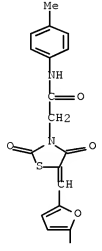
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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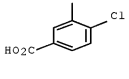
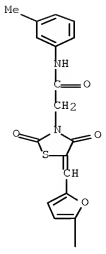


RN 431885-49-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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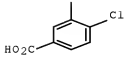
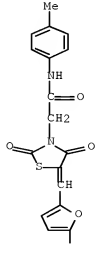


RN 431914-42-0 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 431938-97-5 CAPLUS
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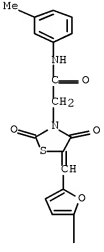
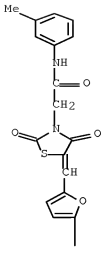
PAGE 1-A



PAGE 2-A

RN 432017-78-2 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

L19 ANSWER 5 OF 10 USPATFULL on STN

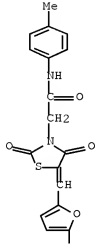
ACCESSION NUMBER:	2007:224298 USPATFULL Full-text			
TITLE:	Immunomodulatory compounds that target and inhibit the py'binding site of tyrosene kinase p56 lck sh2 domain			
INVENTOR(S):	Mackerell, Alexander, Baltimore, MD, UNITED STATES Hayashi, Jun, Ellicott City, MD, UNITED STATES Nagarsekar, Ashish, Gaithersburg, MD, UNITED STATES Huang, Niu, San Francisco, CA, UNITED STATES Macias, Alba, Cambridge, UNITED KINGDOM			
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 20070196395	A1	20070823	
APPLICATION INFO.:	US 2003-582640	A1	20031212	(10)
	WO 2003-US39501		20031212	
			20070420	PCT 371 date
DOCUMENT TYPE:	Utility			
FILE SEGMENT:	APPLICATION			
LEGAL REPRESENTATIVE:	MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON BLVD., SUITE 1400, ARLINGTON, VA, 22201, US			
NUMBER OF CLAIMS:	23			
EXEMPLARY CLAIM:	1			
NUMBER OF DRAWINGS:	2 Drawing Page(s)			
LINE COUNT:	2189			

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Small molecular-weight non-peptidic compounds block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 496767-24-9
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)
RN 496767-24-9 USPATFULL
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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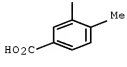


L19 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:1291759 CAPLUS Full-text
DOCUMENT NUMBER: 146:180013
TITLE: Multiplexed Detection of Protein-Peptide Interaction and Inhibition Using Capillary Electrophoresis
AUTHOR(S): Yang, Peilin; Whelan, Rebecca J.; Mao, Yingwei; Lee, Angel W.-M.; Carter-Su, Christin; Kennedy, Robert T.
CORPORATE SOURCE: Department of Chemistry and Department of Pharmacology, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Analytical Chemistry (2007), 79(4), 1690-1695
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English

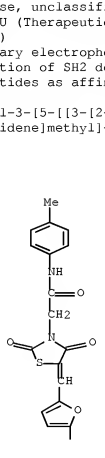
AB High-speed capillary electrophoresis (CE) was employed to detect binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes. Single SH2 protein-phosphopeptide complexes were detected and confirmed by competition and fluorescence anisotropy. The assay was then extended to a multiplexed system involving separation of three SH2 domain proteins: Src, SH2-Bβ, and Fyn. The selectivity of the separation was improved by altering the charge of the peptide binding partners used, thus demonstrating a convenient way to control resolution for the multiplexed assay. The separation was completed within 6 s, allowing rapidly dissociating complexes to be detected. Two low mol. weight inhibitors were tested for inhibition selectivity and efficacy. One inhibitor interrupted binding interaction of all three proteins, while the other selectively inhibited Src only leaving SH2-Bβ and Fyn complex barely affected. IC50 of both selective and nonselective inhibitors were determined and compared for different proteins. The IC50 of the nonselective inhibitor was 49±9, 323±42, and 228±19 μM (n = 3) for Src, SH2-Bβ, and Fyn, resp., indicating different efficacy of the nonselective inhibitor for different SH2 domain protein. It is concluded that high-speed CE has the potential for multiplexed screening of drugs that disrupt protein-protein interactions.

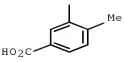
IT 496767-24-9
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(high-speed capillary electrophoresis for multiplexed detection of binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2006:1342378 CAPLUS Full-text
DOCUMENT NUMBER: 146:68774
TITLE: Anti-viral compositions comprising heterocyclic substituted phenyl furans and related compounds
INVENTOR(S): Jiang, Shibo; Debnath, Asim Kumar; Lu, Hong
PATENT ASSIGNEE(S): New York Blood Center, USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287319	A1	20061221	US 2006-448439	20060606
CA 2608821	A1	20061228	CA 2006-2608821	20060606
WO 2006138118	A2	20061228	WO 2006-US21993	20060606
WO 2006138118	A3	20070726		
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
EP 1896033	A2	20080312	EP 2006-772346	20060606
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
JP 2008543836	T	20081204	JP 2008-516935	20060606

PRIORITY APPLN. INFO.: US 2005-691120P P 20050615
WO 2006-US21993 W 20060606

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:68774

AB A group of compds. that inhibit HIV replication by blocking HIV entry was identified. One representative compound, designated NB-206, and its analogs inhibited HIV replication (p24 production) with IC50 values at nanomolar levels. It was proved that NB-206 and its analogs are HIV entry inhibitors by targeting the HIV gp41 since: (1) they inhibited HIV-mediated cell fusion; (2) they inhibited HIV replication only when they were added to the cells less

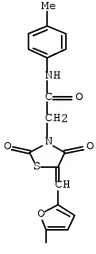
than one hour after virus addition; (3) they blocked the formation of the gp41 core that is detected by sandwich enzyme linked immunosorbent assay (ELISA) using a conformation-specific MAb NC-1; and (4) they inhibited the formation of the gp41 six-helix bundle revealed by fluorescence native-PAGE (FN-PAGE). These results suggested that NB-206 and its analogs may interact with the hydrophobic cavity and block the formation of the fusion-active gp41 coiled coil domain, resulting in inhibition of HIV-1 mediated membrane fusion and virus entry.

IT 430470-21-6 431075-18-2 431883-68-0
431883-95-3 431885-49-3 431914-42-0
431938-97-5 431986-92-4 432017-78-2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-viral compns. comprising heterocyclic substituted Ph furans and related compds.)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 431075-18-2 CAPLUS

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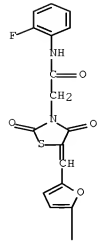
PAGE 1-A



PAGE 2-A

RN 431883-68-0 CAPLUS
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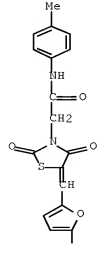
PAGE 1-A



PAGE 2-A

RN 431883-95-3 CAPLUS
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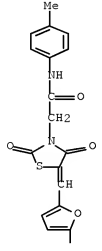
PAGE 1-A



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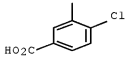

RN 431885-49-3 CAPLUS
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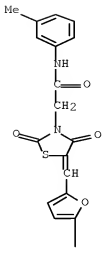
PAGE 1-A



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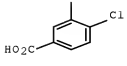

RN 431914-42-0 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

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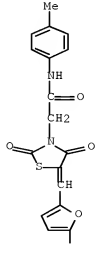
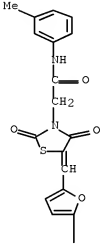


PAGE 2-A

RN 431938-97-5 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 431986-92-4 CAPLUS
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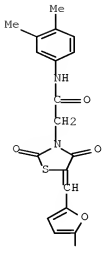
PAGE 1-A



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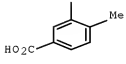
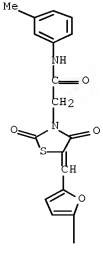


RN 432017-78-2 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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L19 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:588651 CAPLUS Full-text
DOCUMENT NUMBER: 143:109784
TITLE: Immunomodulatory compounds that target and inhibit the py+3 binding site of tyrosine kinase p561ck SH2 domain
INVENTOR(S): Mackerell, Alexander D., Jr.; Hayashi, Jun; Nagarsekar, Ashish; Huang, Niu; Macias, Alba
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA
SOURCE: PCT Int. Appl., 213 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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WO 2005060956	A1	20050707	WO 2003-US39501	20031212
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003297904	A1	20050714	AU 2003-297904	20031212
US 20070196395	A1	20070823	US 2007-582640	20070420

PRIORITY APPLN. INFO.: WO 2003-US39501 A 20031212
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:109784

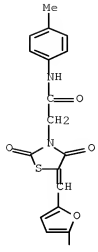
AB Small mol.-wt. non-peptidic compds. block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

IT 496767-24-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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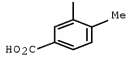


OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1046388 CAPLUS Full-text
DOCUMENT NUMBER: 143:398889
TITLE: Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p56lck
AUTHOR(S): Macias, Alba T.; Mia, Md. Younus; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Chemical Information and Modeling (2005), 45(6), 1759-1766
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Compd. selection based on chem. similarity has been used to validate active "parent" compds. identified via database searching as viable lead compds. and to obtain initial structure-activity relationships for those leads. Twelve parent compds. that have inhibitory activity against the SH2 domain of the p56 T-cell tyrosine kinase (Lck) are the focus of this study. Lck is involved in the T-cell mediated immune response, and inhibitors of Lck protein-protein

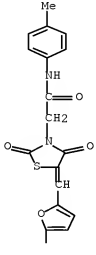
interactions could potentially be used to develop novel immunosuppressants. Similarity searches for each parent compound were performed using 2D structural fingerprints on a database containing 1 300 000 com. available compds. The inhibitory activity of the selected compds. was assessed using enzyme immunoassay (EIA). In general, the most active parent compds. yield the most high activity similar compds.; however, in two cases low activity parent compds. (i.e.inhibitory activity < 25% at 100 μM) yielded multiple similar compds. with activities > 60%. Such compds. may, therefore, be considered as viable lead compds. for optimization. Structure-activity relationships were explored by examining both ligand structures and their computed bound conformations to the protein. Functional groups common to the active compds. as well as key amino acid residues that form hydrogen bonds with the active compds. were identified. This information will act as the basis for the rational optimization of the lead compds.

IT 430470-21-6 430471-43-5 431075-18-2
431883-95-3 431885-49-3 432017-78-2
496767-24-9 591745-24-3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lead validation and SAR development via chemical similarity searching; application to compds. targeting pY+3 site of p56lck SH2 domain)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RN 430471-43-5 CAPLUS

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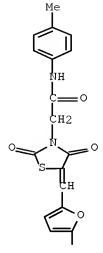
PAGE 1-A



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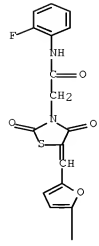

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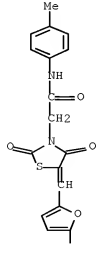

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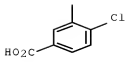

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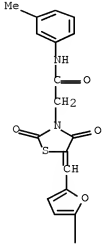

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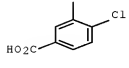

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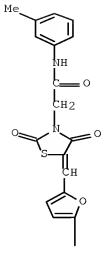
PAGE 1-A



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RN 496767-24-9 CAPLUS
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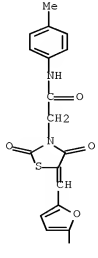
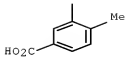
PAGE 1-A





RN 591745-24-3 CAPLUS
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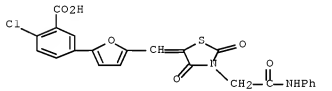


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:453664 CAPLUS Full-text
DOCUMENT NUMBER: 141:98930
TITLE: Identification of non-phosphate-containing small molecular weight inhibitors of the tyrosine kinase p56 Lck SH2 domain via in silico screening against the pY + 3 binding site
AUTHOR(S): Huang, Niu; Nagarsekar, Ashish; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(14), 3502-3511
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The protein p56 lymphoid T cell tyrosine kinase (Lck) is predominantly expressed in T lymphocytes where it plays a critical role in T-cell-mediated immune response. Lck participates in phosphotyrosine-dependent protein-protein interactions through its modular binding unit, the Src homol.-2 (SH2) domain. Accordingly, virtual screening methods combined with exptl. assays were used to identify small mol. weight nonpeptidic compds. that block Lck SH2 domain-dependent interactions. Virtual screening included scoring normalization procedures and postdocking structural clustering that is shown to facilitate the selection of active compds. By targeting the well-defined hydrophobic binding pocket known to impart specificity on Lck-protein interactions (i.e., pY + 3 site), inhibitors of the Lck SH2 domain were

discovered that omit the phosphotyrosine (pY) or related moieties. The 34 out of 196 computationally selected compds. were shown to inhibit Lck SH2 domain association with phosphorylated immunoreceptor tyrosine based activation motifs peptide. Twenty-four of the active compds. were further tested for their ability to modulate biol. function. Thirteen of these compds. showed inhibitory activity in mixed lymphocyte culture assay. Fluorescence titration expts. on four of these active compds. further verified their binding to the SH2 domain. Because of their simple chemical structures, these small organic compds. have the potential to act as lead compds. for the development of novel immunosuppressant drugs.

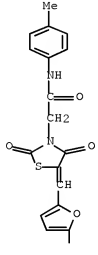
IT 496767-24-9

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of non-phosphate-containing small mol. weight inhibitors of tyrosine kinase p56 Lck SH2 domain via in silico screening against pY + 3 binding site)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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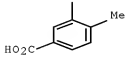

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REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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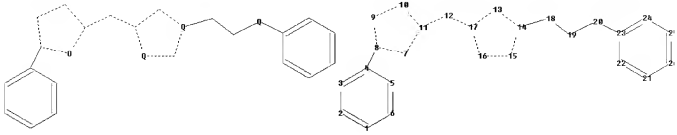

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ring bonds :
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Match level :
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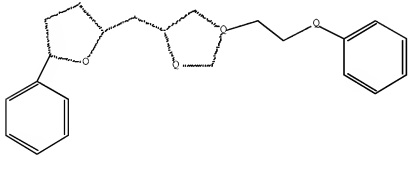

Structure attributes must be viewed using STN Express query preparation.

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STRUCTURE FILE UPDATES:   26 DEC 2010  HIGHEST RN 1257513-11-3
DICTIONARY FILE UPDATES:  26 DEC 2010  HIGHEST RN 1257513-11-3

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http://www.cas.org/support/stngen/stndoc/properties.html

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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
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PROJECTED ITERATIONS:        44635 TO    50485
PROJECTED ANSWERS:             528 TO     1350

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SEARCH TIME: 00.00.01

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CA INDEXING COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)
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PROCESSING COMPLETED FOR L23
L24             5 DUP REMOVE L23 (2 DUPLICATES REMOVED)

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L24  ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2009:489075  CAPLUS Full-text
DOCUMENT NUMBER:          152:287197
TITLE:                    Synthesis and in vivo anticancer and antiangiogenic
                          effects of novel thioxothiazolidin-4-one derivatives
                          against transplantable mouse tumor
AUTHOR(S):                Chandrappa, S.; Chandru, H.; Sharada, A. C.; Vinaya,
                          K.; Ananda Kumar, C. S.; Thimmegowda, N. R.;
                          Nagegowda, P.; Karuna Kumar, M.; Rangappa, K. S.
CORPORATE SOURCE:         Department of Studies in Chemistry, University of
                          Mysore, Mysore, 570006, India
SOURCE:                   Medicinal Chemistry Research (2010), 19(3), 236-249
                          CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER:                Birkhaeuser Boston
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 152:287197
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AB A series of novel thioxothiazolidin-4-one derivs. were synthesized by the coupling of different amines containing aliphatic, substituted aromatic, and heterocyclic moieties, such as oxadiazol, pyrazole, isoxazole, and piperazine with 2-(5-(4-chlorophenyl)furan-2-yl)methylene-4-oxo-2- thioxothiazolidin-3-ylacetic acid. All compds. were characterized by 1H NMR, LCMS, FTIR, and elemental anal. In this study, we investigated the possibility that these novel thioxothiazolidin-4-one derivs. inhibits tumor growth and tumor induced angiogenesis using mouse Ehrlich Ascites Tumor (EAT) as a model system. Our results demonstrated that the compds. significantly reduced ascites tumor volume, cell number, and increased the life span of EAT-bearing mice. In addition, the compds. manifested strong antiangiogenic effects and suppressed tumor induced endothelial proliferation in the mice peritoneum. From our findings, it is noted that some of the derivs. may be possible candidates for anticancer therapy with the ability to inhibit tumor angiogenesis and tumor cell proliferation.

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IT   1160931-81-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (preparation and in vivo anticancer and antiangiogenic effects of
        thioxothiazolidin-4-one derivs. against mouse Ehrlich ascites tumor)
RN   1160931-81-6  CAPLUS
CN   3-Thiazolidineacetamide, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-N-[4-
     (5-methyl-1,2,4-oxadiazol-3-yl)phenyl]-4-oxo-2-thioxo-  (CA INDEX NAME)
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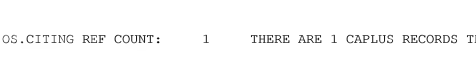


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(1 CITINGS)
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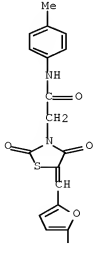
L24 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:581012 CAPLUS Full-text
DOCUMENT NUMBER: 149:69549
TITLE: Discovery of a novel submicromolar inhibitor of the lymphoid specific tyrosine phosphatase
AUTHOR(S): Xie, Yuli; Liu, Yidong; Gong, Gangli; Rinderspacher, Alison; Deng, Shi-Xian; Smith, Deborah H.; Toebben, Udo; Tzilianos, Effie; Branden, Lars; Vidovic, Dusica; Chung, Caty; Schurer, Stephan; Tautz, Lutz; Landry, Donald W.
CORPORATE SOURCE: Department of Medicine, Columbia University, New York, NY, 10032, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2840-2844
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:69549

AB We report here a class of thiazolidine-2,4-diones and 2-thioxothiazolidin-4-ones as potent inhibitors of the lymphoid specific tyrosine phosphatase (Lyp) identified from high throughput screens. Chemical modification by incorporating the known phosphotyrosine (pTyr) mimics led to the discovery of a salicylate-based inhibitor with submicromolar potency.

IT 431883-68-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thiazolidinediones and thioxothiazolidinones as inhibitors of lymphoid specific tyrosine phosphatase)

RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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L24 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2007:484949 CAPLUS Full-text
DOCUMENT NUMBER: 146:475681
TITLE: Immunomodulatory heterocyclic compounds that target and inhibit the pY binding site of tyrosine kinase p56lck SH2 domain
INVENTOR(S): Mackerell, Alexander; Hayashi, Jun
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA
SOURCE: U.S. Pat. Appl. Publ., 90 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070099970	A1	20070503	US 2006-507038	20060821
WO 2008024759	A2	20080228	WO 2007-US76402	20070821
WO 2008024759	A3	20081030		

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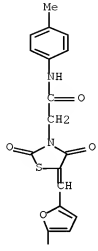
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-709972P P 20050819
US 2006-507038 A 20060821

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:475681
AB Small mol.-wt. non-peptidic compds. block lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.
IT 430470-21-6 431883-68-0 431938-97-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory heterocyclic compound inhibitors of pY binding site of tyrosine kinase p56lck SH2 domain)
RN 430470-21-6 CAPLUS
CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-

thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

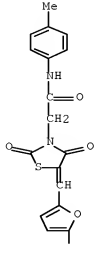
PAGE 1-A



PAGE 2-A

RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

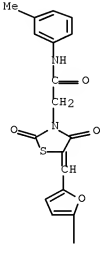
PAGE 1-A



PAGE 2-A

RN 431938-97-5 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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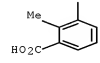

L24 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2006:1342378 CAPLUS Full-text
DOCUMENT NUMBER: 146:68774
TITLE: Anti-viral compositions comprising heterocyclic substituted phenyl furans and related compounds
INVENTOR(S): Jiang, Shibo; Debnath, Asim Kumar; Lu, Hong
PATENT ASSIGNEE(S): New York Blood Center, USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp.

CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287319	A1	20061221	US 2006-448439	20060606
CA 2608821	A1	20061228	CA 2006-2608821	20060606
WO 2006138118	A2	20061228	WO 2006-US21993	20060606
WO 2006138118	A3	20070726		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

EP 1896033	A2	20080312	EP 2006-772346	20060606
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JP 2008543836	T	20081204	JP 2008-516935	20060606
PRIORITY APPLN. INFO.:			US 2005-691120P P	20050615
			WO 2006-US21993 W	20060606

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 146:68774

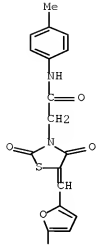
AB A group of compds. that inhibit HIV replication by blocking HIV entry was identified. One representative compound, designated NB-206, and its analogs inhibited HIV replication (p24 production) with IC50 values at nanomolar levels. It was proved that NB-206 and its analogs are HIV entry inhibitors by targeting the HIV gp41 since: (1) they inhibited HIV-mediated cell fusion; (2) they inhibited HIV replication only when they were added to the cells less than one hour after virus addition; (3) they blocked the formation of the gp41 core that is detected by sandwich enzyme linked immunosorbent assay (ELISA) using a conformation-specific MAb NC-1; and (4) they inhibited the formation of the gp41 six-helix bundle revealed by fluorescence native-PAGE (FN-PAGE). These results suggested that NB-206 and its analogs may interact with the hydrophobic cavity and block the formation of the fusion-active gp41 coiled coil domain, resulting in inhibition of HIV-1 mediated membrane fusion and virus entry.

IT 430470-21-6 431883-68-0 431938-97-5
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-viral compns. comprising heterocyclic substituted Ph furans and related compds.)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

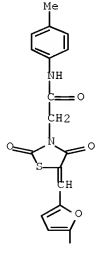
PAGE 1-A



PAGE 2-A

RN 431883-68-0 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

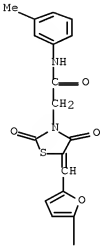
PAGE 1-A



PAGE 2-A

RN 431938-97-5 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L24 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1046388 CAPLUS Full-text
DOCUMENT NUMBER: 143:398889
TITLE: Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p56lck
AUTHOR(S): Macias, Alba T.; Mia, Md. Younus; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of

Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Chemical Information and Modeling (2005), 45(6), 1759-1766
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

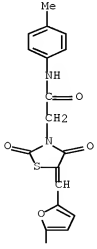
AB Compd. selection based on chem. similarity has been used to validate active "parent" compds. identified via database searching as viable lead compds. and to obtain initial structure-activity relationships for those leads. Twelve parent compds. that have inhibitory activity against the SH2 domain of the p56 T-cell tyrosine kinase (Lck) are the focus of this study. Lck is involved in the T-cell mediated immune response, and inhibitors of Lck protein-protein interactions could potentially be used to develop novel immunosuppressants. Similarity searches for each parent compound were performed using 2D structural fingerprints on a database containing 1 300 000 com. available compds. The inhibitory activity of the selected compds. was assessed using enzyme immunoassay (EIA). In general, the most active parent compds. yield the most high activity similar compds.; however, in two cases low activity parent compds. (i.e.inhibitory activity < 25% at 100 μM) yielded multiple similar compds. with activities > 60%. Such compds. may, therefore, be considered as viable lead compds. for optimization. Structure-activity relationships were explored by examining both ligand structures and their computed bound conformations to the protein. Functional groups common to the active compds. as well as key amino acid residues that form hydrogen bonds with the active compds. were identified. This information will act as the basis for the rational optimization of the lead compds.

IT 430470-21-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lead validation and SAR development via chemical similarity searching; application to compds. targeting pY+3 site of p56lck SH2 domain)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3 4 S SSS FULL L1

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L5 7 DUP REMOVE L4 (2 DUPLICATES REMOVED)
L6 STRUCTURE UPLOADED

FILE 'REGISTRY' ENTERED AT 17:42:18 ON 27 DEC 2010
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L8 4 S L6 SSS FULL
L9 0 S L8 NOT L3
L10 4 S L8 OR L3
L11 STRUCTURE UPLOADED
L12 6 S L11
L13 91 S L11 SSS FULL

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L17 2 S L15 NOT L3
L18 13 S L13
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L20 STRUCTURE UPLOADED

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PROCESSING COMPLETED FOR L25

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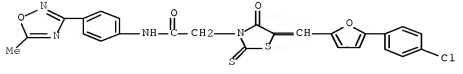
L26 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:489075 CAPLUS Full-text
DOCUMENT NUMBER: 152:287197
TITLE: Synthesis and in vivo anticancer and antiangiogenic effects of novel thioxothiazolidin-4-one derivatives against transplantable mouse tumor
AUTHOR(S): Chandrappa, S.; Chandru, H.; Sharada, A. C.; Vinaya, K.; Ananda Kumar, C. S.; Thimmegowda, N. R.; Nagegowda, P.; Karuna Kumar, M.; Rangappa, K. S.
CORPORATE SOURCE: Department of Studies in Chemistry, University of Mysore, Mysore, 570006, India
SOURCE: Medicinal Chemistry Research (2010), 19(3), 236-249 CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 152:287197

AB A series of novel thioxothiazolidin-4-one derivs. were synthesized by the coupling of different amines containing aliphatic, substituted aromatic, and heterocyclic moieties, such as oxadiazol, pyrazole, isoxazole, and piperazine with 2-(5-(4-chlorophenyl)furan-2-yl)methylene-4-oxo-2- thioxothiazolidin-3-ylacetic acid. All compds. were characterized by 1H NMR, LCMS, FTIR, and elemental anal. In this study, we investigated the possibility that these novel thioxothiazolidin-4-one derivs. inhibits tumor growth and tumor induced angiogenesis using mouse Ehrlich Ascites Tumor (EAT) as a model system. Our results demonstrated that the compds. significantly reduced ascites tumor volume, cell number, and increased the life span of EAT-bearing mice. In addition, the compds. manifested strong antiangiogenic effects and suppressed tumor induced endothelial proliferation in the mice peritoneum. From our findings, it is noted that some of the derivs. may be possible candidates for anticancer therapy with the ability to inhibit tumor angiogenesis and tumor cell proliferation.

IT 1160931-81-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and in vivo anticancer and antiangiogenic effects of thioxothiazolidin-4-one derivs. against mouse Ehrlich ascites tumor)

RN 1160931-81-6 CAPLUS
CN 3-Thiazolidineacetamide, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-N-[4-(5-methyl-1,2,4-oxadiazol-3-yl)phenyl]-4-oxo-2-thioxo- (CA INDEX NAME)



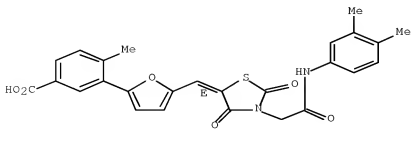
OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2009:875997 CAPLUS Full-text
DOCUMENT NUMBER: 151:115085
TITLE: Method using lifespan-altering compounds for altering the lifespan of eukaryotic organisms, and screening for such compounds
INVENTOR(S): Goldfarb, David Scott
PATENT ASSIGNEE(S): University of Rochester, USA
SOURCE: U.S. Pat. Appl. Publ., 57pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 20
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20090163545	A1	20090625	US 2008-341615	20081222
US 20090163545	A1	20090625	US 2008-341615	20081222
AU 2008345225	A1	20090709	AU 2008-345225	20081222
CA 2709784	A1	20090709	CA 2008-2709784	20081222
EP 2219646	A2	20100825	EP 2008-867410	20081222
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, AL, BA, MK, RS				

PRIORITY APPLN. INFO.: US 2008-23801P P 20080125
US 2007-16362P P 20071221
US 2008-341615 20081222
WO 2008-US88016 W 20081222
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
AB The invention discloses a method for altering the lifespan of a eukaryotic organism. The method comprises the steps of providing a lifespan-altering compound, and administering an effective amount of the compound to a eukaryotic organism, such that the lifespan of the organism is altered. In one embodiment, the compound is identified using the DeaD assay. [This abstract record is one of 20 records for this document necessitated by the large number of index entries required to fully index the document and publication system constraints.]
IT 1164479-41-7
RL: PAC (Pharmacological activity); BIOL (Biological study)
(method using lifespan-altering compds. for altering lifespan of eukaryotic organisms, and screening for such compds.)
RN 1164479-41-7 CAPLUS
CN Benzoic acid, 3-[5-[(E)-[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)

Double bond geometry as shown.



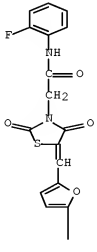
L26 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:1412560 CAPLUS Full-text
DOCUMENT NUMBER: 152:135695
TITLE: Identification of novel agonists of the integrin CD11b/CD18
AUTHOR(S): Faridi, Mohd. Hafeez; Maiguel, Dony; Barth, Constantinos J.; Stoub, Darren; Day, Ruth; Schurer, Stephan; Gupta, Vineet
CORPORATE SOURCE: Peggy and Harold Katz Family Drug Discovery Center, Division of Nephrology and Hypertension, Department of Medicine, University of Miami, Miami, FL, 33176, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2009), 19(24), 6902-6906
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We report the identification of novel small mol. agonists of integrin CD11b/CD18, which increased, in a dose-dependent manner, the adhesion of the integrin CD11b/CD18 expressing cells to two physiol. relevant ligands: Fibrinogen and iC3b. Compound 6 showed an ex vivo EC50 of 10.5 μM and in vitro selectivity for binding to the recombinant αA-domain of CD11b/CD18. In silico docking expts. suggest that the compds. recognized a hydrophobic cleft in the ligand-binding αA-domain, implying an allosteric mechanism of modulation of integrin affinity by this novel compound

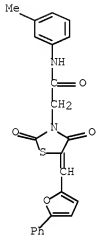
IT 431927-57-0 432020-72-9
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of novel agonists of integrin CD11b/CD18)

RN 431927-57-0 CAPLUS
CN 3-Thiazolidineacetamide, 5-[[5-(2,4-dichlorophenyl)-2-furanyl]methylene]-N-(2-fluorophenyl)-2,4-dioxo- (CA INDEX NAME)

PAGE 1-A



RN 432020-72-9 CAPLUS
CN 3-Thiazolidineacetamide, N-(3-methylphenyl)-2,4-dioxo-5-[(5-phenyl-2-furanyl)methylene]- (CA INDEX NAME)



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2009:825465 CAPLUS Full-text
DOCUMENT NUMBER: 151:235704
TITLE: Identification of Novel Falcipain-2 Inhibitors as Potential Antimalarial Agents through Structure-Based Virtual Screening
AUTHOR(S): Li, Honglin; Huang, Jin; Chen, Lili; Liu, Xiaofeng; Chen, Tong; Zhu, Jin; Lu, Weiqiang; Shen, Xu; Li, Jian; Hilgenfeld, Rolf; Jiang, Hualiang
CORPORATE SOURCE: School of Pharmacy, East China University of Science and Technology, Shanghai, 200237, Peop. Rep. China
SOURCE: Journal of Medicinal Chemistry (2009), 52(15), 4936-4940
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The SPECS database was screened against falcipain-2 with two different docking methods to identify structurally diverse nonpeptidic inhibitors. Twenty-eight nonpeptidic mols. among 81 compds. tested were identified as potential inhibitors of falcipain-2. One of the inhibitors exhibited in vitro activity with an IC50 value of 2.4 μM. Furthermore, the similarity anal. has demonstrated that it is feasible to find novel diverse falcipain-2 inhibitors

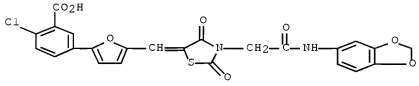
with similar steric shape through virtual screening of large-scale chemical libraries.

IT 592540-03-9 1176856-67-9

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of novel falcipain-2 inhibitors as potential antimalarial agents through virtual screening)

RN 592540-03-9 CAPLUS

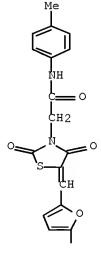
CN Benzoic acid, 5-[5-[[3-[2-(1,3-benzodioxol-5-ylamino)-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-2-chloro- (CA INDEX NAME)



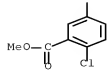
RN 1176856-67-9 CAPLUS

CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-, methyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2009:352002 CAPLUS Full-text

DOCUMENT NUMBER: 150:530312

TITLE: Synthesis of 2-(5-((5-(4-chlorophenyl)furan-2-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid derivatives and evaluation of their cytotoxicity and induction of apoptosis in human leukemia cells

AUTHOR(S): Chandrappa, S.; Kavitha, C. V.; Shahabuddin, M. S.; Vinaya, K.; Ananda Kumar, C. S.; Ranganatha, S. R.; Raghavan, Sathees C.; Rangappa, K. S.

CORPORATE SOURCE: Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore, 570 006, India

SOURCE: Bioorganic & Medicinal Chemistry (2009), 17(6), 2576-2584
CODEN: BMECEP; ISSN: 0968-0896

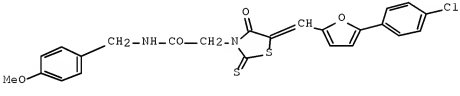
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 150:530312

GI



I

AB In order to explore the anticancer effect assocd. with the thiazolidinone framework, several 2-(5-((5-(4-chlorophenyl)furan-2-yl)methylene)-4-oxo-2-thioxothiazolidin-3-yl)acetic acid derivs. 5(a-l) were synthesized. Variation in the functional group at C-terminal of the thiazolidinone led to set of compds. bearing amide moiety. Their chemical structures were confirmed by 1H NMR, IR and Mass Spectra anal. These thiazolidinone compds. containing furan moiety exhibits moderate to strong antiproliferative activity in a cell cycle stage-dependent and dose dependent manner in two different human leukemia cell lines. The importance of the electron donating groups on thiazolidinone moiety was confirmed by MTT and Trypan blue assays and it was concluded that the 4th position of the substituted aryl ring plays a dominant role for its anticancer property. Among the synthesized compds., 5e (I) and 5f have shown potent anticancer activity on both the cell lines tested. To rationalize the role of electron donating group in the induction of cytotoxicity we have chosen two mols. (5e and 5k) having different electron donating group at different positions. LDH assay, Flow cytometric anal. and DNA fragmentation suggest that 5e is more cytotoxic and able to induce the apoptosis.

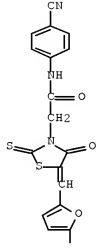
IT 1152541-43-9P 1152541-48-4P

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(furanyl thioxothiazolidines cytotoxic in human leukemia cells)

RN 1152541-43-9 CAPLUS

CN 3-Thiazolidineacetamide, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-N-(4-cyanophenyl)-4-oxo-2-thioxo- (CA INDEX NAME)

PAGE 1-A

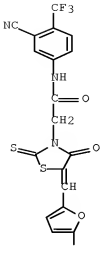


PAGE 2-A

RN 1152541-48-4 CAPLUS

CN 3-Thiazolidineacetamide, 5-[[5-(4-chlorophenyl)-2-furanyl]methylene]-N-[3-cyano-4-(trifluoromethyl)phenyl]-4-oxo-2-thioxo- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)
REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:581012 CAPLUS Full-text
DOCUMENT NUMBER: 149:69549
TITLE: Discovery of a novel submicromolar inhibitor of the lymphoid specific tyrosine phosphatase
AUTHOR(S): Xie, Yuli; Liu, Yidong; Gong, Gangli; Rinderspacher, Alison; Deng, Shi-Xian; Smith, Deborah H.; Toebben, Udo; Tzilianos, Effie; Branden, Lars; Vidovic, Dusica; Chung, Caty; Schurer, Stephan; Tautz, Lutz; Landry, Donald W.
CORPORATE SOURCE: Department of Medicine, Columbia University, New York, NY, 10032, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2008), 18(9), 2840-2844
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:69549
AB We report here a class of thiazolidine-2,4-diones and 2-thioxothiazolidin-4-ones as potent inhibitors of the lymphoid specific tyrosine phosphatase (Lyp)

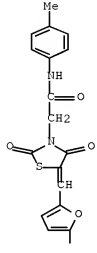
identified from high throughput screens. Chemical modification by incorporating the known phosphotyrosine (pTyr) mimics led to the discovery of a salicylate-based inhibitor with submicromolar potency.

IT 431883-68-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thiazolidinediones and thioxothiazolidinones as inhibitors of lymphoid specific tyrosine phosphatase)

RN 431883-68-0 CAPLUS

CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 2008:823862 CAPLUS Full-text

DOCUMENT NUMBER: 149:323031

TITLE: Combating the Threat of Anthrax: A Quantitative Structure-Activity Relationship Approach

AUTHOR(S): Verma, Rajeshwar P.; Hansch, Corwin

CORPORATE SOURCE: Department of Chemistry, Pomona College, Claremont, CA, 91711, USA

SOURCE: Molecular Pharmaceutics (2008), 5(5), 745-759

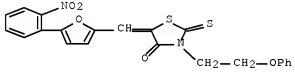
CODEN: MPOHBP; ISSN: 1543-8384
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Bacterial agents or products more likely to be used as biol. weapons of mass destruction are Bacillus anthracis, Francisella tularensis, Yersinia pestis, and the neurotoxin of Clostridium botulinum. Anthrax is an acute infectious disease with a high mortality rate caused by Bacillus anthracis, reinforcing the need for better adjunctive therapy and prevention strategies. In this paper, we developed 7 QSAR models on penicillin-based inhibitors of the class A and B β-lactamases from B. anthracis and inhibitors of anthrax lethal factor to understand the chemical-biol. interactions. Hydrophobic and steric factors are found to be the most important determinants of the activity. Internal (cross-validation (q2), quality factor (Q), Fischer statistics (F), and Y-randomization) and external validation tests have validated all the QSAR models.

IT 1048648-94-7
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(QSAR approach to treating anthrax)

RN 1048648-94-7 CAPLUS

CN 4-Thiazolidinone, 5-[[5-(2-nitrophenyl)-2-furanyl]methylene]-3-(2-phenoxyethyl)-2-thioxo- (CA INDEX NAME)



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REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:723693 CAPLUS Full-text
DOCUMENT NUMBER: 149:252062
TITLE: Pharmacophore modelling and virtual screening for identification of new Aurora-A kinase inhibitors
AUTHOR(S): Deng, Xiao-Qiang; Wang, Hui-Yuan; Zhao, Ying-Lan; Xiang, Ming-Li; Jiang, Pei-Du; Cao, Zhi-Xing; Zheng, Yu-Zhu; Luo, Shi-Dong; Yu, Luo-Ting; Wei, Yu-Quan; Yang, Sheng-Yong
CORPORATE SOURCE: State Key Laboratory of Biotherapy and Cancer Center, West China Hospital West China Medical School, Sichuan University, Sichuan, 610041, Peop. Rep. China
SOURCE: Chemical Biology & Drug Design (2008), 71(6), 533-539
CODEN: CBDDAL; ISSN: 1747-0277
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

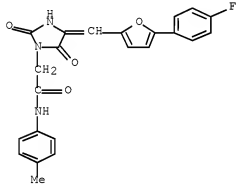
AB Aurora-A has been identified as one of the most attractive targets for cancer therapy and a considerable number of Aurora-A inhibitors have been reported recently. In order to clarify the essential structure-activity relationship for the known Aurora-A inhibitors as well as identify new lead compds. against

Aurora-A, 3D pharmacophore models were developed based on the known inhibitors. The best hypothesis, Hypo1, was used to screen mol. structural databases, including Specs and China Natural Products Database for potential lead compds. The hit compds. were subsequently subjected to filtering by Lipinski's rules and docking study to refine the retrieved hits and as a result to reduce the rate of false pos. Finally, 39 compds. were purchased for further in vitro assay against several human tumor cell lines including A549, MCF-7, HepG2 and PC-3, in which Aurora-A is overexpressed. Two compds. show very low micromolar inhibition potency against some of these tumor cells. And they have been selected for further investigation.

IT 444556-41-6
RL: PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacophore modeling and virtual screening for identification of new Aurora-A kinase inhibitors)

RN 444556-41-6 CAPLUS

CN 1-Imidazolidineacetamide, 4-[[5-(4-fluorophenyl)-2-furanyl]methylene]-N-(4-methylphenyl)-2,5-dioxo- (CA INDEX NAME)



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REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2007:484949 CAPLUS Full-text

DOCUMENT NUMBER: 146:475681

TITLE: Immunomodulatory heterocyclic compounds that target and inhibit the pY binding site of tyrosine kinase p56lck SH2 domain

INVENTOR(S): Mackerell, Alexander; Hayashi, Jun

PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA

SOURCE: U.S. Pat. Appl. Publ., 90 pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070099970	A1	20070503	US 2006-507038	20060821
WO 2008024759	A2	20080228	WO 2007-US76402	20070821

WO 2008024759 A3 20081030

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: US 2005-709972P P 20050819
US 2006-507038 A 20060821

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 146:475681

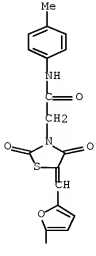
AB Small mol.-wt. non-peptidic compds. block lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

IT 430470-21-6 430471-43-5 431054-19-2
431075-18-2 431075-21-7 431883-68-0
431883-95-3 431885-49-3 431914-42-0
431938-97-5 432017-78-2
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory heterocyclic compound inhibitors of pY binding site of tyrosine kinase p56lck SH2 domain)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

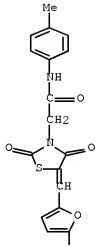
PAGE 1-A



PAGE 2-A

RN 430471-43-5 CAPLUS
CN Benzoic acid, 2-chloro-4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

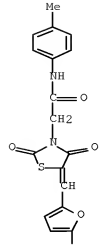
PAGE 1-A



PAGE 2-A

RN 431054-19-2 CAPLUS
CN Benzoic acid, 4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-, methyl ester (CA INDEX NAME)

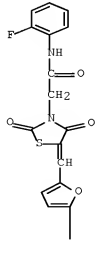
PAGE 1-A



PAGE 2-A

RN 431075-18-2 CAPLUS
CN Benzoic acid, 3-[5-[[3-[2-[(2-fluorophenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-2-methyl- (CA INDEX NAME)

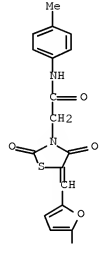
PAGE 1-A



PAGE 2-A

RN 431075-21-7 CAPLUS
CN Benzoic acid, 3-methyl-4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-, methyl ester (CA INDEX NAME)

PAGE 1-A



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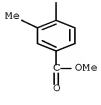

RN 431883-68-0 CAPLUS
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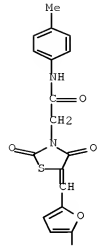
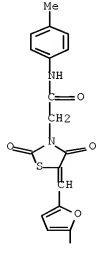
PAGE 1-A



PAGE 2-A

RN 431883-95-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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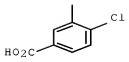
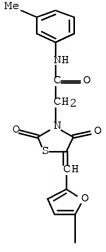


RN 431885-49-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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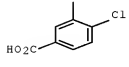
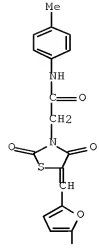


RN 431914-42-0 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

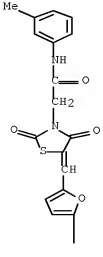
PAGE 1-A



PAGE 2-A

RN 431938-97-5 CAPLUS
CN Benzoic acid, 2-methyl-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

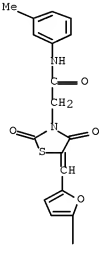
PAGE 1-A



PAGE 2-A

RN 432017-78-2 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

L26 ANSWER 10 OF 15 USPATFULL on STN
ACCESSION NUMBER: 2007:224298 USPATFULL Full-text
TITLE: Immunomodulatory compounds that target and inhibit the py'binding site of tyrosene kinase p56 lck sh2 domain
INVENTOR(S): Mackerell, Alexander, Baltimore, MD, UNITED STATES
Hayashi, Jun, Ellicott City, MD, UNITED STATES
Nagarsekar, Ashish, Gaithersburg, MD, UNITED STATES
Huang, Niu, San Francisco, CA, UNITED STATES
Macias, Alba, Cambridge, UNITED KINGDOM

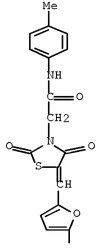
	NUMBER	KIND	DATE	
PATENT INFORMATION:	US 20070196395	A1	20070823	
APPLICATION INFO.:	US 2003-582640	A1	20031212	(10)
	WO 2003-US39501		20031212	
			20070420	PCT 371 date

DOCUMENT TYPE: Utility
FILE SEGMENT: APPLICATION
LEGAL REPRESENTATIVE: MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON BLVD., SUITE 1400, ARLINGTON, VA, 22201, US
NUMBER OF CLAIMS: 23
EXEMPLARY CLAIM: 1
NUMBER OF DRAWINGS: 2 Drawing Page(s)
LINE COUNT: 2189
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Small molecular-weight non-peptidic compounds block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT 496767-24-9
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)
RN 496767-24-9 USPATFULL
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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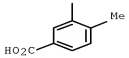
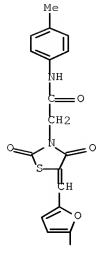


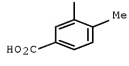
L26 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2006:1291759 CAPLUS Full-text
DOCUMENT NUMBER: 146:180013
TITLE: Multiplexed Detection of Protein-Peptide Interaction and Inhibition Using Capillary Electrophoresis
AUTHOR(S): Yang, Peilin; Whelan, Rebecca J.; Mao, Yingwei; Lee, Angel W.-M.; Carter-Su, Christin; Kennedy, Robert T.
CORPORATE SOURCE: Department of Chemistry and Department of Pharmacology, University of Michigan, Ann Arbor, MI, 48109-1055, USA
SOURCE: Analytical Chemistry (2007), 79(4), 1690-1695
CODEN: ANCHAM; ISSN: 0003-2700
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB High-speed capillary electrophoresis (CE) was employed to detect binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes. Single SH2 protein-phosphopeptide complexes were detected and confirmed by competition and fluorescence anisotropy. The assay was then extended to a multiplexed system involving separation of three SH2 domain proteins: Src, SH2-Bβ, and Fyn. The selectivity of the separation was improved by altering the charge of the peptide binding partners used, thus demonstrating a convenient way to control resolution for the multiplexed assay. The separation was completed within 6 s, allowing rapidly dissociating complexes to be detected. Two low mol. weight inhibitors were tested for inhibition selectivity and efficacy. One inhibitor interrupted binding interaction of all three proteins, while the other selectively inhibited Src only leaving SH2-Bβ and Fyn complex barely affected. IC50 of both selective and nonselective inhibitors were determined and compared for different proteins. The IC50 of the nonselective inhibitor was 49±9, 323±42, and 228±19 μM (n = 3) for Src, SH2-Bβ, and Fyn, resp., indicating different efficacy of the nonselective inhibitor for different SH2 domain protein. It is concluded that high-speed CE has the potential for multiplexed screening of drugs that disrupt protein-protein interactions.

IT 496767-24-9
RL: BUU (Biological use, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(high-speed capillary electrophoresis for multiplexed detection of binding and inhibition of SH2 domain proteins using fluorescently labeled phosphopeptides as affinity probes)

RN 496767-24-9 CAPLUS
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)





OS.CITING REF COUNT: 15 THERE ARE 15 CAPLUS RECORDS THAT CITE THIS RECORD (15 CITINGS)
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2006:1342378 CAPLUS Full-text
DOCUMENT NUMBER: 146:68774
TITLE: Anti-viral compositions comprising heterocyclic substituted phenyl furans and related compounds
INVENTOR(S): Jiang, Shibo; Debnath, Asim Kumar; Lu, Hong
PATENT ASSIGNEE(S): New York Blood Center, USA
SOURCE: U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060287319	A1	20061221	US 2006-448439	20060606
CA 2608821	A1	20061228	CA 2006-2608821	20060606
WO 2006138118	A2	20061228	WO 2006-US21993	20060606
WO 2006138118	A3	20070726		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD,
SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ,
VC, VN, ZA, ZM, ZW
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EP 1896033 A2 20080312 EP 2006-772346 20060606
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IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
BA, HR, MK, YU

JP 2008543836 T 20081204 JP 2008-516935 20060606
PRIORITY APPLN. INFO.: US 2005-691120P P 20050615
WO 2006-US21993 W 20060606

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): MARPAT 146:68774

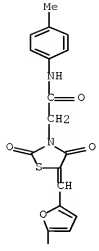
AB A group of compds. that inhibit HIV replication by blocking HIV entry was identified. One representative compound, designated NB-206, and its analogs inhibited HIV replication (p24 production) with IC50 values at nanomolar levels. It was proved that NB-206 and its analogs are HIV entry inhibitors by targeting the HIV gp41 since: (1) they inhibited HIV-mediated cell fusion; (2) they inhibited HIV replication only when they were added to the cells less than one hour after virus addition; (3) they blocked the formation of the gp41 core that is detected by sandwich enzyme linked immunosorbent assay (ELISA) using a conformation-specific MAb NC-1; and (4) they inhibited the formation of the gp41 six-helix bundle revealed by fluorescence native-PAGE (FN-PAGE). These results suggested that NB-206 and its analogs may interact with the hydrophobic cavity and block the formation of the fusion-active gp41 coiled coil domain, resulting in inhibition of HIV-1 mediated membrane fusion and virus entry.

IT 430470-21-6 431075-18-2 431883-68-0
431883-95-3 431885-49-3 431914-42-0
431938-97-5 431986-92-4 432017-78-2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anti-viral compns. comprising heterocyclic substituted Ph furans and related compds.)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

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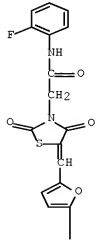
PAGE 1-A



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RN 431883-68-0 CAPLUS
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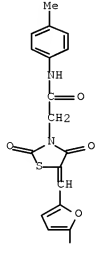
PAGE 1-A



PAGE 2-A

RN 431883-95-3 CAPLUS
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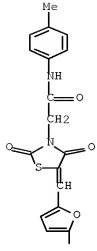
PAGE 1-A



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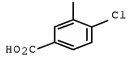
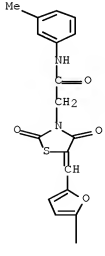


RN 431885-49-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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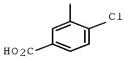

RN 431914-42-0 CAPLUS
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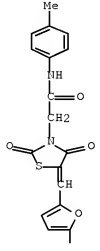
PAGE 1-A



PAGE 2-A

RN 431938-97-5 CAPLUS
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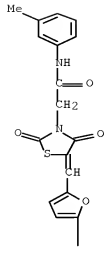
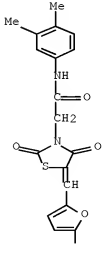
PAGE 1-A



PAGE 2-A

RN 431986-92-4 CAPLUS
CN Benzoic acid, 3-[5-[[3-[2-[(3,4-dimethylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-4-methyl- (CA INDEX NAME)

PAGE 1-A



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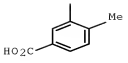
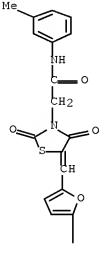


RN 432017-78-2 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L26 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:588651 CAPLUS Full-text
DOCUMENT NUMBER: 143:109784
TITLE: Immunomodulatory compounds that target and inhibit the py+3 binding site of tyrosine kinase p56lck SH2 domain
INVENTOR(S): Mackerell, Alexander D., Jr.; Hayashi, Jun; Nagarsekar, Ashish; Huang, Niu; Macias, Alba
PATENT ASSIGNEE(S): University of Maryland, Baltimore, USA

SOURCE: PCT Int. Appl., 213 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005060956	A1	20050707	WO 2003-US39501	20031212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003297904	A1	20050714	AU 2003-297904	20031212
US 20070196395	A1	20070823	US 2007-582640	20070420

PRIORITY APPLN. INFO.: WO 2003-US39501 A 20031212
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 143:109784

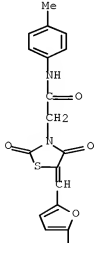
AB Small mol.-wt. non-peptidic compds. block Lck SH2 domain-dependent interactions. The inhibitors omit phosphotyrosine (pY) or related moieties.

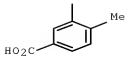
IT 496767-24-9
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(immunomodulatory compds. that target and inhibit py+3 binding site of tyrosine kinase p56 lck SH2 domain)

RN 496767-24-9 CAPLUS

CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L26 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2005:1046388 CAPLUS Full-text
DOCUMENT NUMBER: 143:398889
TITLE: Lead Validation and SAR Development via Chemical Similarity Searching; Application to Compounds Targeting the pY+3 Site of the SH2 Domain of p561ck
AUTHOR(S): Macias, Alba T.; Mia, Md. Younus; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Chemical Information and Modeling (2005), 45(6), 1759-1766
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

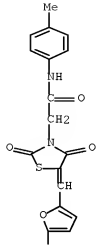
AB Compd. selection based on chem. similarity has been used to validate active "parent" compds. identified via database searching as viable lead compds. and to obtain initial structure-activity relationships for those leads. Twelve parent compds. that have inhibitory activity against the SH2 domain of the p56 T-cell tyrosine kinase (Lck) are the focus of this study. Lck is involved in the T-cell mediated immune response, and inhibitors of Lck protein-protein interactions could potentially be used to develop novel immunosuppressants. Similarity searches for each parent compound were performed using 2D structural fingerprints on a database containing 1 300 000 com. available compds. The inhibitory activity of the selected compds. was assessed using enzyme immunoassay (EIA). In general, the most active parent compds. yield the most high activity similar compds.; however, in two cases low activity parent compds. (i.e.inhibitory activity < 25% at 100 μM) yielded multiple similar compds. with activities > 60%. Such compds. may, therefore, be considered as viable lead compds. for optimization. Structure-activity relationships were explored by examining both ligand structures and their computed bound conformations to the protein. Functional groups common to the active compds. as well as key amino acid residues that form hydrogen bonds with the active compds. were identified. This information will act as the basis for the rational optimization of the lead compds.

IT 430470-21-6 430471-43-5 431054-19-2
431075-18-2 431075-21-7 431883-95-3
431885-49-3 432017-78-2 496767-24-9
591745-24-3 867335-66-8
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lead validation and SAR development via chemical similarity searching; application to compds. targeting pY+3 site of p561ck SH2 domain)

RN 430470-21-6 CAPLUS

CN Benzoic acid, 3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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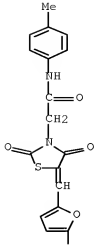
RN 430471-43-5 CAPLUS
CN Benzoic acid, 2-chloro-4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

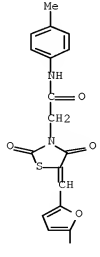
PAGE 1-A



PAGE 2-A

RN 431054-19-2 CAPLUS
CN Benzoic acid, 4-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-, methyl ester (CA INDEX NAME)

PAGE 1-A



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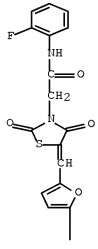
RN 431075-18-2 CAPLUS
CN Benzoic acid, 3-[5-[[3-[2-[(2-fluorophenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



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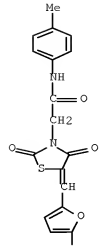
PAGE 1-A



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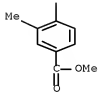
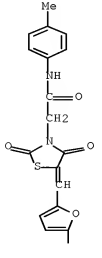


RN 431883-95-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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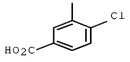
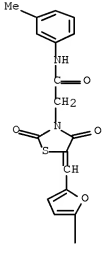


RN 431885-49-3 CAPLUS
CN Benzoic acid, 4-chloro-3-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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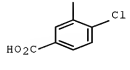

RN 432017-78-2 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[3-[2-[(3-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

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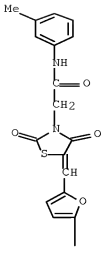

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RN 496767-24-9 CAPLUS
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

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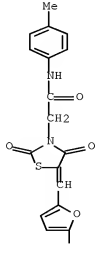
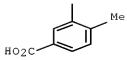
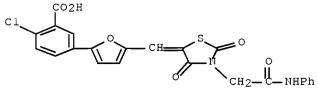




RN 591745-24-3 CAPLUS
CN Benzoic acid, 2-chloro-5-[5-[[2,4-dioxo-3-[2-oxo-2-(phenylamino)ethyl]-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)



RN 867335-66-8 CAPLUS
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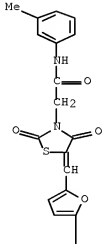
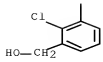




OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (4 CITINGS)
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

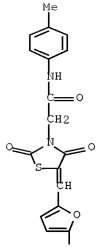
L26 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:453664 CAPLUS Full-text
DOCUMENT NUMBER: 141:98930
TITLE: Identification of non-phosphate-containing small molecular weight inhibitors of the tyrosine kinase p56 Lck SH2 domain via in silico screening against the pY + 3 binding site
AUTHOR(S): Huang, Niu; Nagarsekar, Ashish; Xia, Guanjun; Hayashi, Jun; MacKerell, Alexander D., Jr.
CORPORATE SOURCE: Department of Pharmaceutical Sciences, School of Pharmacy, University of Maryland, Baltimore, MD, 21201, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(14), 3502-3511
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The protein p56 lymphoid T cell tyrosine kinase (Lck) is predominantly expressed in T lymphocytes where it plays a critical role in T-cell-mediated immune response. Lck participates in phosphotyrosine-dependent protein-protein interactions through its modular binding unit, the Src homol.-2 (SH2) domain. Accordingly, virtual screening methods combined with exptl. assays were used to identify small mol. weight nonpeptidic compds. that block Lck SH2 domain-dependent interactions. Virtual screening included scoring normalization procedures and postdocking structural clustering that is shown to facilitate the selection of active compds. By targeting the well-defined hydrophobic binding pocket known to impart specificity on Lck-protein interactions (i.e., pY + 3 site), inhibitors of the Lck SH2 domain were discovered that omit the phosphotyrosine (pY) or related moieties. The 34 out of 196 computationally selected compds. were shown to inhibit Lck SH2 domain association with phosphorylated immunoreceptor tyrosine based activation motifs peptide. Twenty-four of the active compds. were further tested for their ability to modulate biol. function. Thirteen of these compds. showed inhibitory activity in mixed lymphocyte culture assay. Fluorescence titration expts. on four of these active compds. further verified their binding to the SH2 domain. Because of their simple chemical structures, these small organic compds. have the potential to act as lead compds. for the development of novel immunosuppressant drugs.

IT 496767-24-9
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(identification of non-phosphate-containing small mol. weight inhibitors of tyrosine kinase p56 Lck SH2 domain via in silico screening against pY + 3 binding site)

RN 496767-24-9 CAPLUS
CN Benzoic acid, 4-methyl-3-[5-[[3-[2-[(4-methylphenyl)amino]-2-oxoethyl]-2,4-dioxo-5-thiazolidinylidene]methyl]-2-furanyl]- (CA INDEX NAME)

PAGE 1-A



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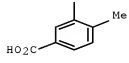

OS.CITING REF COUNT: 51 THERE ARE 51 CAPLUS RECORDS THAT CITE THIS RECORD (53 CITINGS)
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 18:02:33 ON 27 DEC 2010